

Discovery of Novel Complex Metal Hydrides for Hydrogen Storage through Molecular Modeling and Combinatorial Methods (New FY 2004 Project)

Dr. David Lesch

UOP Research Department

25 E. Algonquin Road

Des Plaines, IL. 60017-5017

Phone: (847) 391-3894; Fax: (847) 391-3550; E-mail: dalesch@uop.com

DOE Technology Development Manager: Carole Read

Phone: (202) 586-3152; Fax: (202) 586-9811; E-mail: Carole.Read@ee.doe.gov

Objectives

To discover complex metal hydrides for hydrogen storage that contain 6% or more of hydrogen and can reversibly desorb hydrogen between -40 and 90°C

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year R,D&D Plan:

- A. Cost
- B. Weight and Volume
- M. Hydrogen Capacity and Reversibility

Approach

The objective of the proposed project is to discover complex metal hydrides for hydrogen storage which contain 6% or more of hydrogen and can reversibly desorb hydrogen between -40 and 90°C. The project will combine molecular modeling with high-throughput combinatorial material synthesis, testing and characterization, large-scale materials testing, and system engineering studies to produce prototype commercially viable hydrogen storage systems.

The focus of the first project year is to establish, validate and demonstrate the combinatorial tools and molecular modeling approach, while initiating materials discovery experiments. Specific first year objectives include:

- Refine technical requirements

- Develop and validate medium-throughput (parallel) synthesis, screening and characterization tools
- Design and implement the high-throughput solution and solid-phase synthesis, screening and characterization tools
- Develop theoretical methods to predict equilibrium structures of complex hydrides
- Finalize material classes for the second year screening studies
- Begin screening experiments on complex metal hydrides in the medium-throughput system

The focus throughout the second year will include screening studies of candidate hydrogen storage materials. Screening will continue in the medium-throughput system while validating the high-throughput system, after which both systems will be used. Detailed modeling and characterization studies will guide screening toward materials likely to have thermodynamics required to meet the DOE

technical targets. Modeling and characterization and the results from the screening studies will be used to identify mechanisms of action in new materials.

Specific second year objectives include:

- Validate the high-throughput synthesis and testing system
- Perform screening studies (medium and high throughputs) on expanded classes of complex metal hydrides
- Perform modeling studies to predict the thermodynamics of novel complex hydrides
- Conduct detailed characterization studies on promising candidates
- Advance mechanistic understanding of new complex metal hydrides
- Evaluate and select most promising classes/candidates for optimization studies in the third year

The goal of the third project year is to produce an economical hydrogen storage system by optimizing hydride catalyst combinations, scaling them up for commercial testing, and performing analyses to assess the economic value of the resulting hydrogen storage system. Specific third year objectives include:

- Predict phase diagrams of candidate materials from empirical data and theoretical predictions
- Optimize hydride/catalyst combinations
- Demonstrate successful scale-up and design prototype hydrogen storage systems
- Conduct engineering analyses to verify suitability to meet DOE technical targets
- Analyze economic factors to establish commercial viability